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FUNDAMENTAL INFORMATION FOR TIGER CODE CALCULATIONS ON EXPLOSIVES (1)

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FUNDAMENTAL INFORMATION FOR TIGER CODE CALCULATIONS ON EXPLOSIVES (1)

by

D.E.G. Jones* and K.K. Feng*

SUMMARY

The thermodynamic information required in the TIGER computer code for the components of an explosive composition and for the expected detonation products are discussed. The source of this information is outlined, and the effect of variation in some of these properties on predicted detonation parameters is given. A new, complete and accurate compilation of fitted C_p data for 42 gaseous detonation products is presented.

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INFORMATION ESSENTIELLE POUR EFFECTUER DES CALCULS EN CODE TIGER SUR LES EXPLOSIFS (1)

par

D.E.G. Jones* et K.K. Feng*

RÉSUMÉ

On étudie dans ce rapport l'information thermodynamique requise pour le code machine TIGER servant aux éléments de composition d'un explosif ainsi qu'aux produits destinés à détoner. On souligne également la source de cette information et donne l'effet de la variation chez certaines de ces propriétés sur les paramètres de détonation prévus. Une nouvelle compilation complète et précise des données C_p convenant à 42 produits de détonation gazeux est aussi présentée dans ce rapport.

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INTRODUCTION

Reliable and accurate prediction of detonation properties such as velocity, pressure and temperature is fundamental to advances in explosive science. Development of a computer code for this purpose has been an ongoing study in this field. The TIGER code (1), based on a thermodynamic analysis, is one such code and is used extensively in our laboratory. In order to use this code, complete and accurate thermodynamic data for the components of both the explosive composition and the detonation products is required. It is the object of this report to provide some of this information and to illustrate the effects of variations in such data on the predicted detonation parameters.

THE PROBLEM

In the past, calculation of detonation parameters was often done using either roughly estimated or inaccurate experimental thermodynamic data. Frequently, the thermodynamic data were hidden away in a variety of obscure sources and in a variety of units. Occasionally, the wrong data were used as errors were handed down from user to user. This report will endeavour to correct these problems by providing a compilation of the best thermodynamic data available in one collection and in one consistent set of units.

STANDARD ENTHALPY AND ENTROPY OF FORMATION

COMPONENTS OF EXPLOSIVE COMPOSITION

The standard enthalpies and entropies of formation of the components of the explosive composition are used as input data in the TIGER code. From this information, the TIGER code calculates the specific heat and entropy of the composition.

The standard enthalpy of formation, $\Delta_f H°$, of a compound is obtained from: (i) the heat of combustion of that compound; (ii) a heat of reaction involving that compound, wherein the standard enthalpies of formation are known for all the other reactants and products; or (iii) by some method of estimation such as bond energies, etc. (2).

The standard entropy, S°, of a compound may be obtained by integrating heat capacity data (see Part 2) up to the temperature of interest or alternately by an estimation technique as above.

Appendix A is a table which lists values of $\Delta_f H°$ (298.15 K) and S° (298.15 K) for some common components of explosive compositions. Included in this table are values of $\Delta_f U°$ (298.15 K), the standard internal energy of formation, since the latter is used to calculate the heat of explosion. The values of $\Delta_f U°$ (298.15 K) are determined from

$$\Delta_f H° \text{ (298.15)} = \Delta_f U° \text{ (298.15 K)} + P\Delta_f V°$$

where P = 1 atm and $\Delta_f V$ is the volume change on formation of the component in its standard state. In some cases, the effect of the value of $\Delta_f H°$ used on the detonation parameters is significant. An example of such a case is the methylammonium nitrate-water system illustrated in Table 1.

COMPONENTS OF THE DETONATION PRODUCTS

The components of the detonation products are chosen from the TIGER library to be a set of linearly independent constituents. The thermodynamic properties of these constituents are determined from the TIGER code using the standard enthalpy and entropy of formation of the constituents. This information is available from the JANAF tables (3) and/or NBS circulars (4,5). Values of $\Delta_f H°$ (298.15 K) and S° (298.15 K) for a series of 42 gaseous detonation products are given in Appendix B, which also includes $\Delta_f U°$ (298.15 K). Discussion of the condensed components will be deferred to a later report.

HEAT CAPACITY

It is necessary to fit heat capacity data to a functional dependance on temperature, T, in order to determine the thermodynamic properties of the components of the gaseous detonation products. The ideal gas heat capacity data provided in the JANAF tables is used to fit the following functions:

$$C_p/R = \sum_{i=1}^{4} C_i \theta^{i-1} + \sum_{i=5}^{7} C_i \theta^{4-i}$$

where C_p is the heat capacity in cal/mol K and $\theta = T/1000$ with T in K. The values of C_i in this equation are then used to determine coefficients C_8 and C_9 from

$$C_8 = \Delta_f H^\circ\ (298.15\ K) - 298.15RF_1(C_i)$$

where R is the gas constant in cal/mol K and

$$F_1(C_i) = \sum_{i=1}^{4} (C_i X^{i-1}/i) + C_5 X^{-1} \log X - \sum_{i=6}^{7} [C_i X^{4-i}/(4 - i)]$$

and

$$C_9 = S^\circ(298.15\ K) - RF_2(C_i)$$

where

$$F_2(C_i) = C_1 \log X + \sum_{i=2}^{4} [C_i\ X^{i-1}/(i - 1)] - \sum_{i=5}^{7} [C_i\ X^{4-i}/(4 - i)]$$

with $X = 0.29815$. Appendix C lists the values of C_i for i = 1 to 9 for the gaseous detonation products of Appendix B.

Real gas heat capacities can be estimated by a method outlined in Sherwood (2), which relies on an assumed equation of state for the gas and gas mixtures. This method has not as yet been applied to the detonation products of Appendix C.

EQUATION OF STATE OF GASEOUS PRODUCTS

To calculate the thermodynamic properties of the gaseous products, it is necessary to adopt an equation of state (EOS) which adequately describes the gases and their mixtures in the temperature and pressure range expected. Further, the detonation parameters are determined by combining the EOS with the conservation equations from hydrodynamic theory.

In earlier studies, the BKW EOS (6) was used for this purpose. Values of the molecular parameter, called the covolume must be available to use this EOS. The covolume may be empirically determined from PVT data or alternatively estimated by geometrical considerations for each molecule.

More recently, the JC3 EOS (7) has been incorporated into the TIGER code and used to predict detonation properties as well as fume compositions (8). This EOS requires two molecular parameters for each component and the values of these parameters are dependent on the form of the intermolecular potential function chosen. For a given potential function, the manner in which these parameters are determined affects the values of the intermolecular force constants, r^* and ε^*/k, where r^* and ε^* are scaling factors used in the potential function. Thus, a different set of values of r^* and ε^*/k results from the type of experimental data used to determine them. Sherwood et al. (2) give a correlation between critical constants, r^* and ε^* for the Leonard-Jones 12-6 potential, using both second virial coefficient and viscosity data.

A comparison of results for the methylammonium nitrate-water system using both the BKW and JC3 EOS is given in Table 1. The effect of variation in the parameters r^* and ε^*/k on the detonation parameters from the JC3 EOS is also illustrated in this table.

The values of r^* and ε^*/k used in the TIGER library are principally derived from the Leonard Jones 12-6 potential. However, it has been recommended (7) that the 13.5-6 potential function be used to derive r^* and ε^*/k for the JC3 equation. The mathematical technique for carrying out this determination using second virial coefficient data is described by Hirschfelder et al. (9) and will be the subject of future work in this area since the JC3 EOS appears to be one of the most reliable and useful EOS.

CONCLUSION

This report provides a comprehensive list of the best available thermodynamic data for a number of components of explosive compositions and a number of possible gaseous detonation products. The effect of variation in thermodynamic data on the detonation parameters has been illustrated, as has the effect of using different EOS and different molecular parameters for the JC3 EOS. Further, heat capacity data for a series of gaseous detonation products have been fitted to a function of temperature, and the regression coefficients have been tabulated for use in the TIGER library data. Finally, this work has established a number of important projects which are to be done in the future.

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Table 1 - Detonation parameters and composition of detonation products for MEAN/H_2O system at C-J condition

EOS	P/katm	T/K	V/cm^3/g	-E/cal/g	D/km/s
BKW	98	1940	0.5867	2007	5.46
JC3(1)	100	2114	0.6049	2009	5.77
JC3(2)	118	2563	0.5968	1996	6.14
JC3(3)	116	2275	0.6547	1390	7.21
JC3(4)	103	2136	0.6211	2004	6.11

Concentration of component/mol/kg of explosive

Component	BKW	JC3(1)	JC3(2)	JC3(3)	JC3(4)
$H_2O(g)$	25.78	20.04	19.32	6.351	17.18
NH_3	1.095	9.936	10.30	12.10	11.92
CO_2	3.942	7.402	7.503	9.136	8.898
N_2	8.592	4.176	3.993	3.090	3.184
CO	1.532	0.3443	0.8704	0.0015	0.2158
H_2	0.4111	0.1127	0.2294	0.1363	0.0847
CH_4	3.677	0.0657	0.0995	--	0.0277
C_2H_2	0.0022	--	--	--	--
O_2	--	--	--	0.0014	--
NO	--	--	--	0.0020	--
$H_2O(l)$	--	--	--	10.56	--
C(s)	--	1.333	0.6643	--	--

MEAN - Methylammonium nitrate

JC3(1) - $\Delta_f H°$(MEAN, 298.15 K) = -84.7 kcal/mol (4)

JC3(2) - $\Delta_f H°$(MEAN, 298.15 K) = -58.0 kcal/mol (14)

JC3(3) - r^* [$H_2O(g)$] changed from 3.35 [JC3(1)] to 4.35

JC3(4) - ε^*/k [$H_2O(g)$] changed from 138 [JC3(1)] to 300

APPENDIX A

THERMODYNAMIC PROPERTIES OF COMPONENTS OF EXPLOSIVE COMPOSITIONS AT 298.15 K

APPENDIX A

THERMODYNAMIC PROPERTIES OF COMPONENTS OF EXPLOSIVE COMPOSITIONS AT 298.15 K

Component	$\Delta_f H°$/kcal/mol	$\Delta_f U°$/kcal/mol	S°/cal/mol K	Reference
NH_4NO_3	-87.37	-84.76	36.11	4
RDX	14.71	20.04	-	12
TNT	-13.0			14
	-15.4			13
	-15.1	-11.0		11
PETN	-128.7	-121.6		12
$NaNO_3$	-101.54	-100.36	27.85	10
H_2O	-68.315	-67.426	16.71	4
$Ca(NO_3)_2$	-224.0	-222.0	46.2	10
$NaClO_4$	-101.0	-99.5		10
SiO_2	-215.94	-215.35	11.2	4
$NaOOCCH_3$	-170.45	-168.97		10
$C_2H_6O_2$	-108.7	-106.3	39.9	4
$C_6H_{12}O_6$	-68.3	-63.0		10
$C_{96}H_{14}$	-51.0	-47.0		?
Al	0.0	0.0	6.77	4
$CH_3NH_3NO_3$	-58.0			14
	-84.7	-81.4	35.0	4
Tetryl	8.06	13.3		12
$C_5H_{12}O_4$	-230.0	-226.0		?
$N_2C_2H_8O_4$	-96.5	-92.4		?
$C_{10}C_{22}$	-59.67	-53.15		?
$(CH_2)_6N_4$	32.506	37.246		10
NH_4ClO_4	-70.58	-67.62	44.5	4
HNO_3	-41.61	-40.13	37.19	4
$C_{7.17}H_{14}$	-45.0	-40.9		?
CH_3COOH	-115.8	-114.0	38.2	4

APPENDIX B

THERMO PROPERTIES OF GASEOUS DETONATION PRODUCTS

APPENDIX B

THERMODYNAMIC PROPERTIES OF GASEOUS DETONATION PRODUCTS AT 298.15 K

Component	$\Delta_f H°$/kcal/mol	$\Delta_f U°$/kcal/mol	S°/cal/mol K
SiO_2	-73.0	-73.0	54.7
Cl	29.082	28.490	39.457
C_2H_2	54.19	54.19	48.0
OH	9.31	9.31	43.89
SiC	172.0	171.4	50.9
CO_2	-94.051	-94.051	51.06
O_2	0.0	0.0	49.003
CO	-26.416	-26.716	47.219
Na_2	32.67	32.08	54.994
CH_2O	-27.7	-27.4	52.26
NaOH	-50.4	-50.4	56.5
H_2O	-57.796	-57.500	45.104
H_2	0.0	0.0	31.208
Cl_2	0.0	0.0	53.288
NH_3	-11.02	-10.43	45.97
HCl	-22.063	-22.062	44.646
N_2	0.0	0.0	45.77
CH_4	-17.880	-17.288	44.492
NO	21.570	21.570	50.347
Al	78.00	77.41	39.3028
SiO	-24.0	-24.3	50.64
Ca	42.850	42.258	36.992
CaOH	-53.3	-53.3	56.8
AlO	21.80	21.50	52.17
AlO_2	-44.0	-44.0	58.7
Al_2O	-31.0	-31.3	61.96
Al_2O_2	-97.0	-97.0	63.7
O	59.553	58.961	38.467
C	171.291	170.699	37.7597
CaCl	-25.0	-25.3	57.7
$CaCl_2$	-112.7	-112.7	69.3
CH_3	34.82	35.12	46.38

APPENDIX B (cont'd)

Component	$\Delta_f H°$/kcal/mol	$\Delta_f U°$/kcal/mol	S°/cal/mol K
$COCl_2$	-52.6	-52.3	67.816
C_2H_4	12.54	13.13	52.396
CH	142.0	141.7	43.72
CH_2	92.07	92.07	43.27
N_2O	19.61	19.91	52.55
ClO	24.19	24.19	54.145
ClO_2	35.0	35.3	56.8
Cl_2O	21.0	21.3	64.019
NO_2	7.91	8.21	57.34
N	112.979	112.387	36.622

APPENDIX C

VALUES OF C(I), I = 1, 9 AS USED IN THE TIGER LIBRARY

APPENDIX C

VALUES OF C(I), I = 1, 9 AS USED IN THE TIGER LIBRARY

SILICON DIOXIDE

8.872351728, -0.5451187663, 0.09888142558, 0.006585069487, -1.612145288,
0.2078648367, -0.009704724451, -80810.48611861463, 67.68695270203394.

CHLORINE ATOM

2.828143587, -0.2316440935, 0.0548184365, -0.00426249819, 0.05959922808,
-0.03589520432, 0.002689079136, 27199.97091871507, 46.45711191747138.

ACETYLENE

7.812911622, 1.9816268, -0.4056653287, 0.0300580257, -1.287019407,
0.119964164, -0.003605210395, 47056.9571313964, 58.32290471187578.

HYDROXYL RADICAL

2.422141166, 1.179054644, -0.2322700423, 0.01644532983, 0.3587280559,
-0.03664065369, 0.001462596503, 8409.580712216746, 51.05466724246353.

SILICON CARBIDE

2.044861508, 1.191360782, -0.1991157216, 0.01182252541, 2.456873981,
-0.6413870219, 0.04091339554, 172777.4527479407, 65.35828931087536.

CARBON DIOXIDE

8.08704534, 0.06606852148, -0.03634078218, 0.004383022416, -1.839533549,
0.2627001037, -0.01245598446, -101659.9495763331, 60.83655199698592.

OXYGEN

4.781706584, -0.03273512318, 0.05930211832, -0.006683341811, -0.7541344221,
0.137365235, -0.007472972732, -3812.859885342311, 56.83892497142129.

CARBON MONOXIDE

4.176027266, 0.375958726, -0.09321586902, 0.007657182685, -0.5934256399,
0.127621184, -0.007541510978, -29582.69601325391, 54.32993791506095.

DIATOMIC SODIUM

4.49703068, 0.1951962966, -0.0003080401343, 0.00002370371119,
-0.005392041929, 0.0001735395442, 29960.6942358651, 65.65516039387811.

FORMALDEHYDE

9.8819987, 0.8552123049, -0.25068519, 0.02104697594, -3.696156392,
0.6935508858, -0.03836203522, -38321.2794582938, 57.69781701109915.

SODIUM HYDROXIDE

5.71890817, 0.8083598172, -0.1725264067, 0.01240228894, -0.5644681608,
0.07510684163, -0.003590964947, -54753.90024443738, 66.77689072445305.

WATER

3.102872827, 2.312985788, -0.469257166, 0.03341331984, -0.02819113106,
0.04063509621, -0.003106293642, -59662.32220891264, 51.42518094741293.

HYDROGEN

2.035153078, 1.2165561846, 0.01492474943, 0.681527725, -0.1296720052,
0.006707029905, -463.2779257224769, 38.63831611898748.

CHLORINE

4.92013297, -0.2727616723, 0.1089527836, -0.01043464514, -0.2425130078,
0.001665141538, 0.008877394765, -3365.857394623754, 63.89666498015978.

AMMONIA

6.78602458, 2.06499129, -0.4025928033, 0.03139098639, -2.02468183,
0.3921003687, -0.02195413371, -17717.26692486531, 51.44018257331062.

HYDROGEN CHLORIDE

3.053876367, 0.9494798486, -0.2009503618, 0.0149846664, -0.002082742259,
0.02580116561, -0.002017932554, -23807.4144298018, 51.66926570743688.

NITROGEN

3.863896573, 0.5422198899, -0.1293785641, 0.01038974339, -0.4448786783,
0.1025526166, -0.006224300516, -2790.944915159005, 52.77775277430234.

METHANE

10.37054674, 2.528281186, -0.6258025338, 0.04904436582, -4.465696496,
0.8691196439, -0.04887751191, -29730.0337395334, 46.71650112344549.

NITROGEN OXIDE NO

4.603862696, 0.1455342877, -0.04325399941, 0.003905683211, -0.7810346872,
0.1657386434, -0.009497294559, 17950.3233533379, 57.74573383513481.

ALIMINUM GAS

2.300778511, 0.1766970867, -0.06309841682, 0.007689884992, 0.08764301243,
-0.007443906133, 0.00057961542, 76789.89112001135, 45.24933373203591.

SILICON MONOXIDE

5.119741381, -0.1547563441, 0.008709005242, 0.002299743349, -0.8131145549,
0.1337092817, -0.006843724448, -28160.69101085179, 58.94721485637641.

CALCIUM

7.349114833, -3.85850348, 1.122399808, -0.07950137587, -2.353264522,
0.4283183251, -0.02377716642, 35746.71978929333, 45.36234358031492.

CALCIUM MONOHYDROXIDE

6.3602471184, 0.5319211614, -0.07793508401, 0.006206053402, -0.2436228016,
-0.02227630773, 0.002186228433, -57824.02513372401, 69.96918860327446

ALUMINUM OXIDE AlO

0.9863016989, 3.257579336, -0.7835728412, 0.05961153426, 1.192603482,
-0.227595275, 0.01303163049, 22438.16927505299, 58.41076299073573.

ALUMINUM DIOXIDE AlO_2

8.579467503, -0.5047988674, 0.09780642991, -0.005503738547, -1.005082974,
0.07596816667, -0.002038227073, -50974.01156275345, 73.72233891989625.

DIALUMINUM OXIDE Al_2O

8.049212995, -0.4798327713, 0.09582579735, -0.006824831243, -1.004005526,
0.08917812423, -0.003367784233, -37526.23438790636, 75.91474463408487.

DIALUMINUM DIOXIDE Al_2O_2

12.85488581, -1.29213675, 0.256303093, -0.01817078692, -2.776210477,
0.3266490421, -0.013092056, 80.1776892166154.

OXYGEN ATOM

2.60831788, -0.09434787065, 0.02810146802, -0.00169200371, -0.04352374824,
0.02228815203, -0.001541722122, 58042.06835978396, 44.7136908977785.

CARBON GAS

2.558618324, -0.1037033183, 0.0551863205, -0.005291654662, --0.008882853598,
0.0003609950745, 0.00006284696653, 169764.9726051916, 43.91598178505134.

CALCIUM MONOCHLORIDE

5.134845416, -0.4310863651, 0.1304114149, -0.006074577902, -0.3138691167,
0.03197694411, -0.001507387589, -28565.12993619593, 68.52051759818685.

CALCIUM CHLORIDE

7.523359825, -0.01269606005, 0.002758056608, -0.0002064382407,
-0.01587467591, -0.03679566586, 0.002254058716, -117414.7646263847,
86.9394409786124.

METHYL RADICAL

6.683037184, 2.349070234, -0.5370649897, 0.04050176557, -1.700139281,
0.3162735723, -0.01752493735, 38485.5786375665, 52.87221011586173.

PHOSGENE $COCl_2$

11.14974898, -0.03865117203, 0.06156050571, -0.003705008212, -1.659781926,
0.1447598002, -0.004596038426, -62251.28477645463, 85.29393365848269.

ETHYLENE

14.86708005, 1.780131724, -0.4664453225, 0.0371855783, -5.816607981,
0.9852874889, -0.5140520739, -4413.672527665578, 58.09471163393162.

CH RADICAL

1.998901351, 2.064714215, -0.4788886196, 0.03713449906, 0.361275151,
-0.03036267308, 0.0007405176188, 141316.2706185742, 49.43258682984413.

CH_2 RADICAL

6.118465133, 1.276758611, -0.3015880095, 0.02304988342, -1.663442804,
0.3041368845, -0.0165240599, 86179.28129192953, 49.15327234496848.

NITROUS OXIDE N_2O

8.212878222, -0.7201825613, -0.01299033802, 0.002083770095, -1.767018644,
0.246074784, --0.01161377766, 12011.28244976289, 63.02751154977282.

CHLORINE OXIDE ClO

5.052352164, -0.1997216748, 0.05129283067, -0.003668863061, -0.5198945405,
0.05630468321, -0.001962239661, 20316.28833829078, 63.52433142624896.

CHLORINE DIOXIDE ClO_2

8.47302509, -0.5612260068, 0.1265640136, -0.008873089881, -1.496425979,
0.1843204529, -0.007816913705, 27569.52558641221, 69.38906461099631.

DICHLORINE OXIDE Cl_2O

7.58713169, -0.2836563381, 0.05854758866, -0.004258821958, -0.5104946304,
-0.01100891379, 0.002916228912, 15260.18685138533, 78.97549047682482.

NITROGEN DIOXIDE NO_2

8.556480761, -0.5271575689, 0.0835206035, -0.004968339633, -2.181973991,
0.3553225046, -0.01821570877, -197.3197277620188, 67.19544786281539

NITROGEN ATOM

2.736899144, -0.1619834291, 0.03230768621, 0.0008213559794, -0.123743405,
0.023336874, -0.001317651455, 111235.348548938, 42.68820887463894.